Access DB# 280715

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Leah Schlientz Examiner #: [illegible] Date: 12/15/08
Art Unit: 1618 Phone Number 30 2-9928 Serial Number: 10/551,292
Mail Box and Bldg/Room Location: Remsen Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. MG

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Bifunctional tridentate pyrazolyl containing ligands for Re and Tc Tricarbonyl complexes

Inventors (please provide full names): Isabel Santos, Jose Domingos Correia, Antonio Paulo, Susana Alves, Rute Vitor

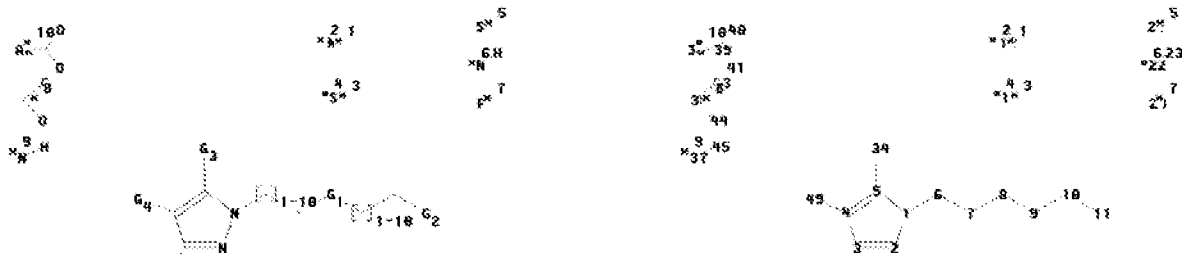
Earliest Priority Filing Date: 4/15/2004

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Structure search
- especially claims
#1, 24, 25, 26, 36, 38
and 50-52.

Structure uploaded into STN REGISTRY

Uploading L1.str



chain nodes :
6 7 8 9 10 11 21 22 23 24 33 34 36 37 38 39 40 41 43 44 45 49

ring nodes :
1 2 3 4 5
ring/chain nodes :
12 13
chain bonds :
1-6 3-33 4-49 5-34 6-7 7-8 8-9 9-10 10-11 22-23 36-43 36-44 37-45 38-39
39-40 39-41
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-6 2-3 3-4 3-33 4-5 4-49 5-34 6-7 7-8 8-9 9-10 10-11 36-43 36-44 37-45 38-39 39-40 39-41
exact bonds :
22-23

G1:[*1-*2],[*3-*4]

G2:[*5],[*6],[*7]

G3:H,Cb,Ak

G4:[*8],[*9],[*10]

Hydrogen count :
3:>= minimum 0
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 33:CLASS 34:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 43:CLASS 44:CLASS 45:CLASS 49:CLASS

Structure search history

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=> d stat query L4
L1              STR

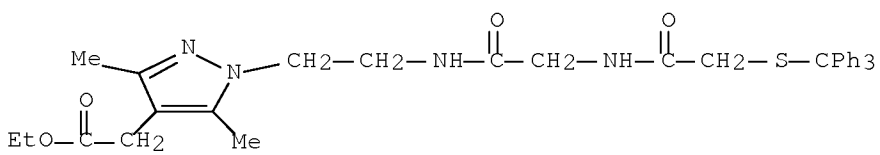
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L3           12 SEA FILE=REGISTRY SSS FUL L1
L4            5 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L3
```

Structure search results

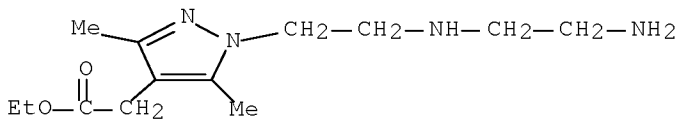
=> d L4 1-5 ibib ed abs hitstr

L4 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:22645 HCAPLUS Full-text
DOCUMENT NUMBER: 146:307704
TITLE: Rhenium(V) oxocomplexes with novel pyrazolyl-based N4- and N3S-donor chelators
AUTHOR(S): Moura, Carolina; Vitor, Rute F.; Maria, Leonor; Paulo, Antonio; Santos, Isabel C.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Dalton Transactions (2006), (47), 5630-5640
CODEN: DTARAF; ISSN: 1477-9226
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:307704
ED Entered STN: 08 Jan 2007
AB The novel pyrazolyl-based ligands 3,5-Me2pz(CH2)2NH(CH2)2NH(CH2)2NH2 (1) and pz*(CH2)2NH-Gly-CH2STrit (pz* = pz (8), 3,5-Me2pz (9), 4-(EtOOC)CH2-3,5-Me2pz (10)) were synthesized, and their suitability to stabilize Re(V) oxocomplexes was evaluated using different starting materials, (NBu4)[ReOCl4], [ReOCl3(PPh3)2] and trans-[ReO2(py)4]Cl. Compound 1 reacts with trans-[ReO2(py)4]Cl yielding the cationic compound [ReO(OMe){3,5-Me2pz(CH2)2N(CH2)2NH(CH2)2NH2}](BPh4) (11) in a low isolated yield. In contrast, the neutral complexes [ReO{pz*(CH2)2NH-Gly-CH2S}] (pz* = pz (12), 3,5-Me2pz (13), 4-(EtOOCCH2)-3,5-Me2pz (14)) were synthesized almost quant. by reacting [ReOCl3(PPh3)2] or (NBu4)[ReOCl4] with the trityl-protected chelators 8-10. The x-ray diffraction anal. of 11 and 13 confirmed the tetradentate coordination mode of the resp. ancillary ligands. In 11 the monoanionic chelator coordinates to the metal through four N atoms, while in 13 the chelator is trianionic, coordinating to the metal through three nitrogens and one S atom. Solution NMR studies of 12-14, including two-dimensional NMR techniques (1H COSY and 1H/13C HSQC), confirmed that the N3S coordination mode of the chelators is retained in solution Unlike 11, complexes 12-14 may be considered relevant in the development of radiopharmaceuticals, as further corroborated by the synthesis of the congener [99mTcO{pz(CH2)2-NH-Gly-CH2S}] (12a). This radioactive compound was obtained from 99mTcO4- in aqueous medium, in almost quant. yield and with high specific activity and radiochem. purity.
IT 927883-71-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with oxorhenate chloro complex)
RN 927883-71-4 HCAPLUS
CN 1H-Pyrazole-4-acetic acid, 3,5-dimethyl-1-[2-[[2-[[2-[(triphenylmethyl)thio]acetyl]amino]acetyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

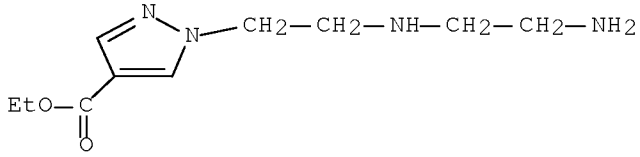


REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1049014 HCAPLUS Full-text
DOCUMENT NUMBER: 142:168330
TITLE: Rhenium(I)- and technetium(I) tricarbonyl complexes anchored by bifunctional pyrazole-diamine and pyrazole-dithioether chelators
AUTHOR(S): Vitor, Rute F.; Alves, Susana; Correia, J. D. G.; Paulo, Antonio; Santos, Isabel
CORPORATE SOURCE: ITN, Estrada Nacional, Departamento de Quimica, Sacavem Codex, 2686-953, Port.
SOURCE: Journal of Organometallic Chemistry (2004), 689(25), 4764-4774
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:168330
ED Entered STN: 08 Dec 2004
AB The novel pyrazolyl containing ligands 4-(HOOC)pz(CH2)2NH(CH2)2NH2 (L1) and 4-(HOOCCH2)-3,5-Me2pz(CH2)2NH(CH2)2NH2 (L2), and 3,5-Me2pz(CH2)2S(CH2)2SCH2CH3 (L3), 3,5-Me2pz(CH2)2S(CH2)2SCH2COOEt (L4) and 3,5-Me2pz(CH2)2S(CH2)2SCH2COOH (L5) were synthesized, and their ability to stabilize complexes with the fac-[M(CO)3]+ (M = Re,99mTc) moiety was evaluated. Reactions of L1-L5 with (NEt4)2[Re(CO)3Br3] and/or [Re(CO)5Br] afforded complexes fac-[Re(CO)3(κ3-L)] (L = L1-L5 (1-5)), which contain the pyrazolyl ancillary ligands coordinated in a tridentate fashion. Complexes 1-5 were characterized by the common anal. techniques, which included single crystal x-ray diffraction anal. in the case of 4. The structural anal. of 4 confirmed the tridentate coordination mode of the pyrazole-dithioether ligand, which is facially coordinated to the Re(I) center through the N from the pyrazole ring and the two thioether S atoms, without involvement of the terminal ester functional group. The distorted octahedral coordination environment around the metal is completed by the three facial carbonyl ligands. The radioactive congeners of complexes 1, 3 and 4, fac-[99mTc(CO)3(κ3-L)]+ (L = L1 (1a), L3 (3a), L4 (4a)), were prepared by reacting the precursor fac-[99mTc(CO)3(H2O)3]+ with the corresponding ligands, and their identity confirmed by HPLC comparison with the Re surrogates. Complexes 1a and 3a were challenged in the presence of a large excess of histidine or cysteine, to evaluate their in vitro stability. Only a negligible displacement was observed, indicating that pyrazole-diamine and pyrazole-dithioether chelators provide a high kinetic inertness and/or stability to organometallic complexes with the fac-[99mTc(CO)3]+ moiety.
IT 827596-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium)
RN 827596-91-8 HCAPLUS
CN 1H-Pyrazole-4-acetic acid, 1-[2-[(2-aminoethyl)amino]ethyl]-3,5-dimethyl-, ethyl ester (CA INDEX NAME)



IT 827596-90-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium and technetium)
RN 827596-90-7 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[(2-aminoethyl)amino]ethyl]-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

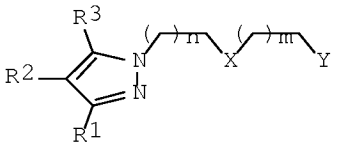
L4 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:902222 HCAPLUS Full-text
DOCUMENT NUMBER: 141:387794
TITLE: Preparation of bifunctional pyrazole-containing tridentate ligands for rhenium and technetium tricarbonyl complexes
INVENTOR(S): Santos, Isabel R.; Galamba Correia, Joao D.; Rocha Paulo, Antonio M.; Alves, Susana; Vitor, Rute
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

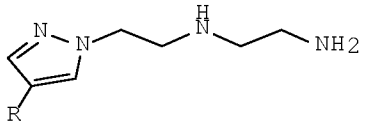
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091669	A1	20041028	WO 2004-US11685	20040415
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1529537	A1	20050511	EP 2003-78217	20031010
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004229568	A1	20041028	AU 2004-229568	20040415
CA 2522326	A1	20041028	CA 2004-2522326	20040415
EP 1644050	A1	20060412	EP 2004-759566	20040415

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

CN 1774268	A	20060517	CN 2004-80010214		20040415
JP 2007525452	T	20070906	JP 2006-510091		20040415
US 20060198785	A1	20060907	US 2005-551292		20050928
IN 2005CN02650	A	20070525	IN 2005-CN2650		20051014
NO 2005005334	A	20051111	NO 2005-5334		20051111
PRIORITY APPLN. INFO.:			EP 2003-76106	A	20030415
			EP 2003-78217	A	20031010
			WO 2004-US11685	W	20040415

OTHER SOURCE(S): MARPAT 141:387794
ED Entered STN: 28 Oct 2004
GI

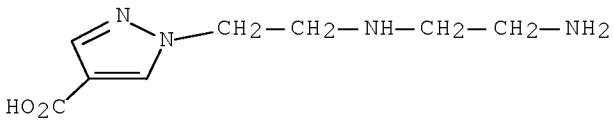

I


II

AB The present invention relates to a chelating agent I [m = 0, 1; X = NR4, S; Y = SR5, NHR5, P(R5)2; R1, R3 = independently H, alkyl, aryl; R2 = H, CO2H, NHR6, (CH2)nCO2R6; R4 = H, alkyl, aryl, (CH2)nCO2R6, (CH2)nOR6; R5 = H, alkyl, aryl, (CH2)nCO2R6, (CH2)nOR6, R6 = H, alkyl, aryl; n = 1-10; when R1 = R3 = CH3, R2, R4, R5 are not all = H]. The invention further relates to a method and kit for the preparation of radiolabeled biomols. while using the chelating agent. Thus, pyrazole II (R = CO2H) was prepared by cyclocondensation of (OHC)2CHCO2Et with H2NNHCH2CH2OH, followed by tosylation and substitution with ethylenediamine and saponification Prepared compds. II (R = H, CO2H) underwent complexation with rhenium and technetium-99 to give the corresponding tricarbonyl complexes.

IT 782501-75-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium and technetium tricarbonyl complexes)

RN 782501-75-1 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[(2-aminoethyl)amino]ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

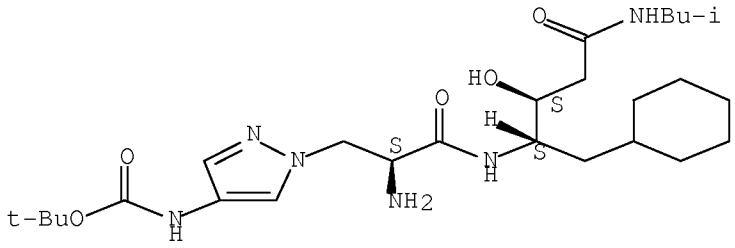
L4 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:591969 HCAPLUS Full-text
DOCUMENT NUMBER: 113:191969
ORIGINAL REFERENCE NO.: 113:32513a,32516a
TITLE: Renin inhibitory peptides containing (4S)-amino-5-cyclohexyl-(3S)-hydroxypentanoic acid
INVENTOR(S): Smith, Stephen Allan; Ham, Peter; Nash, David John
PATENT ASSIGNEE(S): Beecham Group PLC, UK
SOURCE: Eur. Pat. Appl., 91 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

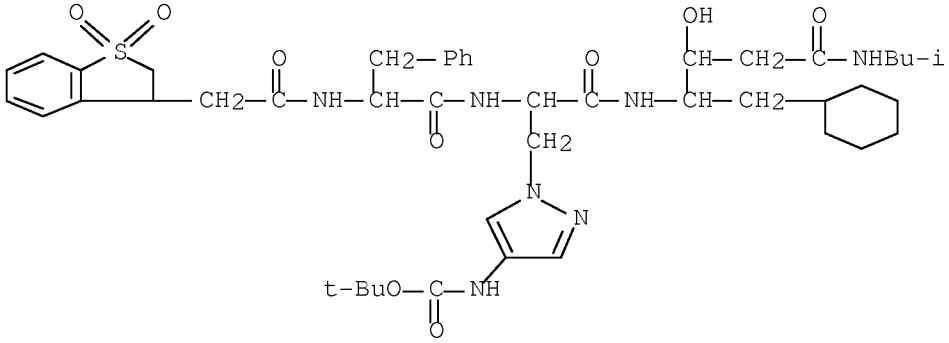
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 350163	A2	19900110	EP 1989-305691		19890606
EP 350163	A3	19901122			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
DK 8902794	A	19891210	DK 1989-2794		19890607
AU 8936121	A	19891214	AU 1989-36121		19890607
ZA 8904301	A	19900530	ZA 1989-4301		19890607
JP 02036169	A	19900206	JP 1989-144298		19890608
PRIORITY APPLN. INFO.:			GB 1988-13671	A	19880609
			GB 1988-29065	A	19881213
			GB 1989-6262	A	19890318

OTHER SOURCE(S): MARPAT 113:191969
ED Entered STN: 23 Nov 1990
GI For diagram(s), see printed CA Issue.
AB The title peptides [I; Z1Z2Z3 = atoms to complete a 5-membered nonarom. heterocyclic ring; E = absent, (CH2)n, CH(CH2)n-1; n = 1-4; A = CONH, NHCO, CO2, CH2, S(O)r; r, p = 0-2; q = 0,1; R1 = (un)substituted (hetero)arylmethyl; R2 = CHR8R9; R8 = H, Me and R9 = C1-6 alkyl, C3-8 cycloalkyl, (un)substituted (hetero)aryl; R9 = NH2, C2-7 alkanoylamino, 2-oxopyrrolidinyl, etc.; R3 = alkyl, cycloalkylmethyl; R4 = (cyclo)alkyl; R5 = H, alkyl; or R5 = OH when A = CH2; R6,R7 = H, substituent], useful for the treatment of hypertension, are prepared Thus, N-(2,3-dihydrobenzofuran-2-carbonyl)-(S)-phenylalanyl-(S)-leucine was condensed with (4S)-amino-5-cyclohexyl-(3S)-hydroxypentanoic acid isobutylamide (ACHPAA) in the presence of hydroxybenzotriazole and DCC in THF at room temperature overnight to give Q-Phe-Leu-ACHPAA (II; Q = 2,3-dihydrobenzofuran-2-carbonyl). II [Q = (6-aminomethyl-2,3-dihydro-1,1-dioxobenzothiophen-3-ylacetyl] in vitro inhibited human renin with an IC50 of 0.8 + 10-8M. A total of 75 I were prepared
IT 130106-44-4P 130106-45-5P 130120-64-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for renin-inhibitory peptide)
RN 130106-44-4 HCAPLUS
CN L-threo-Pentonamide, 4-[[2-amino-3-[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1H-pyrazol-1-yl]-1-oxopropyl]amino]-5-cyclohexyl-2,4,5-trideoxy-N-(2-methylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

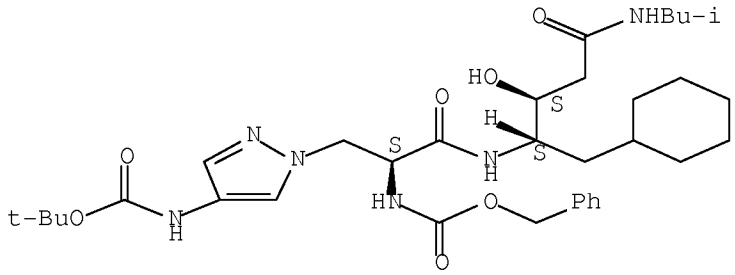


RN 130106-45-5 HCAPLUS
CN L-threo-Pentonamide, 5-cyclohexyl-2,4,5-trideoxy-4-[[N-[N-[(2,3-dihydro-1,1-dioxidobenzo[b]thien-3-yl)acetyl]-L-phenylalanyl]-3-[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1H-pyrazol-1-yl]-L-alanyl]amino]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)



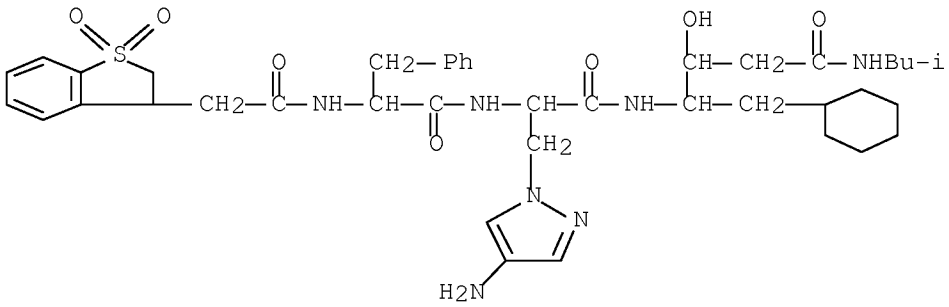
RN 130120-64-8 HCAPLUS
CN L-threo-Pentonamide, 5-cyclohexyl-2,4,5-trideoxy-4-[[3-[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1H-pyrazol-1-yl]-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-N-(2-methylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

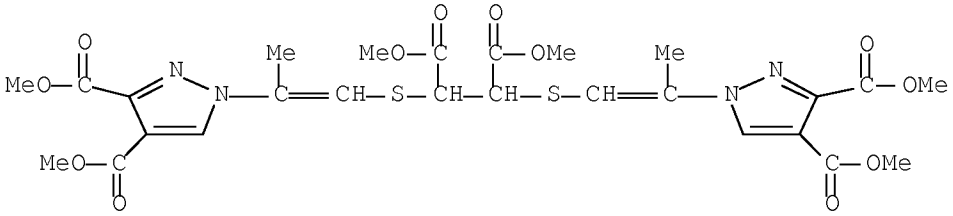


IT 130105-06-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)
(preparation of, as renin inhibitor)
RN 130105-06-5 HCAPLUS
CN L-threo-Pentonamide, 4-[[3-(4-amino-1H-pyrazol-1-yl)-N-[N-[(2,3-dihydro-1,1-dioxidobenzo[b]thien-3-yl)acetyl]-L-phenylalanyl]-L-alanyl]amino]-5-cyclohexyl-2,4,5-trideoxy-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:6272 HCAPLUS Full-text
DOCUMENT NUMBER: 102:6272
ORIGINAL REFERENCE NO.: 102:1139a,1142a
TITLE: New aspects of the 1,3-dipolar cycloaddition of thiazolium N-imines with dimethyl acetylenedicarboxylate (DMAD)
AUTHOR(S): Hirano, Hiroshi; Sugiyama, Kazuaki; Yamashita, Mayumi; Ishida, Toshimasa; Doi, Mitsunobu; Inoue, Masatoshi
CORPORATE SOURCE: Osaka Coll. Pharm., Matsubara, 580, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1984), 32(6), 2446-9
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 Jan 1985
AB 4-Methylthiazolium N-imine reacted with DMAD in MeOH to give 3 products, di-Me [2-[3,4-bis(methoxycarbonyl)-1-pyrazolyl]propenylthio]fumarate, di-Me 2,3-bis[2-[3,4-bis(methoxycarbonyl)-1- pyrazolyl]propenylthio]succinate, and 3-methyl-6-methoxycarbonyl-8-oxidothiazolo[3,2-b]pyridazinium (I). The structure of I was established by x-ray anal. and IR spectral data. In a similar reaction with 4,5-dimethylthiazolium N-imine, 2,3-dimethyl-6,7-bis(methoxycarbonyl)-7,7a-dihydro-4H-thiazolo[3,2- b]pyrazole was isolated, and this compound, when heated in EtOH, underwent ring expansion into an analog of I.
IT 93623-91-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 93623-91-7 HCAPLUS
CN 1H-Pyrazole-3,4-dicarboxylic acid, 1,1'-[[1,2-bis(methoxycarbonyl)-1,2-ethanediyl]bis[thio(1-methyl-2,1-ethenediyl)]]bis-, tetramethyl ester (9CI) (CA INDEX NAME)



Inventor search history

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=> d his L23

     (FILE 'HCAPLUS' ENTERED AT 10:19:08 ON 16 DEC 2008)
L23          14 S L20 OR L22

=> d que L23
L5          483 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  SANTOS I?/AU
L6          527 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  CORREIA J?/AU
L7           91 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  PAULO A?/AU
L8          324 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  ALVES S?/AU
L9           20 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  VITOR R?/AU
L10           2 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L5 AND L6 AND L7 AND
                L8 AND L9
L11          56 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L5 AND (L6 OR L7 OR
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L12          12 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L6 AND (L7 OR L8 OR
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L13           8 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L7 AND (L8 OR L9)
L14           3 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L8 AND L9
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                OR L9)
L16           3 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L15 AND MALLINCKRODT?/
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L19          28 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L17 AND (TRICARBON?
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L22          11 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L18 AND L19
L23          14 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L20 OR L22


=> d que L24
L5          483 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  SANTOS I?/AU
L6          527 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  CORREIA J?/AU
L7           91 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  PAULO A?/AU
L8          324 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  ALVES S?/AU
L9           20 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  VITOR R?/AU
L10           2 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L5 AND L6 AND L7 AND
                L8 AND L9
L24           0 SEA L10


=> d his L24

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L24           0 S L10

=> d his L25

     (FILE 'MEDLINE, BIOSIS, EMBASE, DRUGU' ENTERED AT 10:29:22 ON 16 DEC 2008)
L25          16 S L23

=> d que L25
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L6          527 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  CORREIA J?/AU
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L10           2 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L5 AND L6 AND L7 AND
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L11          56 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L5 AND (L6 OR L7 OR
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L12          12 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L6 AND (L7 OR L8 OR
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L13           8 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L7 AND (L8 OR L9)
L14           3 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L8 AND L9
L15        1366 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L5 OR L6 OR L7 OR L8
                OR L9)
L16           3 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L15 AND MALLINCKRODT?/
                CO,CS,PA,SO
L17          57 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L11 OR L12 OR L13 OR
                L14)
L18          32 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L17 AND PYRAZOL?
L19          28 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L17 AND (TRICARBON?
                OR TRIDENT?)
L20           5 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L10 OR L16
L22          11 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L18 AND L19
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L25          16 SEA L23


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COPYRIGHT (C) 2008 THOMSON REUTERS
PROCESSING COMPLETED FOR L23
PROCESSING COMPLETED FOR L25
L34          15 DUP REM L23 L25 (15 DUPLICATES REMOVED)
                ANSWERS '1-14' FROM FILE HCAPLUS
                ANSWER '15' FROM FILE EMBASE
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Inventor search results

=> d L34 1-15 ibib ab

L34 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2008:521195 HCAPLUS Full-text
TITLE: Pyrazolyl-diamine ligands that bear anthracenyl moieties and their rhenium(I) tricarbonyl complexes: synthesis, characterisation and DNA-binding properties
AUTHOR(S): Vitor, Rute F.; Correia, Isabel; Videira, Margarida; Marques, Fernanda; Paulo, Antonio ; Pessoa, Joao Costa; Viola, Giampietro; Martins, Gabriel G.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: ChemBioChem (2008), 9(1), 131-142
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two novel families of pyrazolyl-diamine ligands that bear an anthracen-9-yl group as a DNA-binding fragment, pz*(CH2)2NH(CH2)2NHCH2-9-anthryl (pz* = pz (L1), 3,5-Me2pz (L2)) and pz*(CH2)2NH(CH2)2NH2 (pz* = 4-(9-anthrylmethyl)pz (L3), 3,5-Me2-4-(9-anthrylmethyl)pz (L4)), have been prepared and fully characterised. In the case of L2-L4, the evaluation of their coordination capability towards the fac-[Re(CO)3]+ core led to the synthesis of the organometallic complexes fac-[Re(CO)3{3,5-Me2pz(CH2)2NH(CH2)2NHCH2-9-anthryl}]Br (7) and fac-[Re(CO)3{4-(9- anthrylmethyl)pz*(CH2)2NH(CH2)2NH2}]Br (pz* = pz (8), 3,5-Me2pz (9)). The interaction of the novel pyrazole-diamine ligands and the rhenium(I) complexes with calf thymus (CT) DNA has been investigated with a variety of spectroscopic techniques (UV-visible, fluorescence, CD (CD) and linear dichroism (LD)). All of the evaluated compds. have a moderate affinity to CT DNA (3.46 + 103 < Kb < 1.95 + 104), but the binding mode depends on the position of the chromophore in the framework of the pyrazolyl-diamine ligands. LD measurements have shown that L1 and L2 act as DNA intercalators, but complex 7 intercalates only partially. By contrast, the compds. with the anthracenyl group at the 4-position of the azolyl ring (L3, L4 and 9) do not intercalate, and behave more like DNA groove binders. Fluorescence microscopy studies have demonstrated that complexes 7 and 9 can target the nucleus of murine B16-F1 melanoma cells, and appear to be promising platforms for the further design of radiopharmaceuticals for targeted radiotherapy.
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2007:749128 HCAPLUS Full-text
DOCUMENT NUMBER: 147:334888
TITLE: Rhenium and technetium tricarbonyl complexes anchored by pyrazole-based tripods: novel lead structures for the design of myocardial imaging agents
AUTHOR(S): Maria, Leonor; Cunha, Susana; Videira, Margarida; Gano, Lurdes; Paulo, Antonio; Santos, Isabel C.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Dalton Transactions (2007), (28), 3010-3019
CODEN: DTARAF; ISSN: 1477-9226
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:334888

AB This report describes the synthesis and biol. evaluation of cationic 99mTc-tricarbonyl complexes anchored by ether-containing tris(pyrazolyl)methane or bis(pyrazolyl)ethanamine ligands to be applied in the design of radiopharmaceuticals for myocardial imaging: fac-[99mTc(CO)3{RC(pz)3}]+ (R = H (1a), MeOCH2 (2a), EtOCH2 (3a), PrOCH2 (4a)) and fac-[99mTc(CO)3{RNHCH2CH(pz)2}]+ (R = H (5a), MeO(CH2)2 (6a)) (pz = pyrazolyl). At the no carrier added level, complexes 1a-6a were obtained in high radiochem. yield (> 98%) by reaction of fac-[99mTc(CO)3(H2O)3]+ with the corresponding tripod chelator in aqueous medium. All these complexes display a high in vitro and in vivo stability, except 6a which metabolizes in vivo yielding fac-[99mTc(CO)3{HO(CH2)2NHCH2CH(pz)2}]+ (7a). Biol. studies in mice showed that among the radiotracers evaluated 3a, anchored by a tris(pyrazolyl)methane chelator bearing an Et Me ether substituent, has the highest heart uptake (3.6 ± 0.5%ID g-1 at 60 min p.i.). Complex 3a presents also the best heart : blood, heart : liver and heart : lung ratios, appearing as the most promising as a potential myocardial imaging agent. The chemical identity of 1a-7a was ascertained by HPLC comparison with the previously reported fac-[Re(CO)3{HC(pz)3}]Br (1) and with the novel fac-[Re(CO)3{RC(pz)3}]Br (R = MeOCH2 (2), EtOCH2 (3), PrOCH2 (4)) and fac-[Re(CO)3{RNHCH2CH(pz)2}]Br (R = H (5), MeO(CH2)2 (6) HO(CH2)2 (7)). The novel Re(I) tricarbonyl complexes 2-7 were characterized by the common anal. techniques, including single crystal x-ray diffraction anal. The solid state structure confirmed the presence of facial and tridentate (κ3-N3) anchor ligands. Solution NMR studies also showed that this κ3-N3 coordination mode is retained in solution for all complexes (2-7).

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2007:605111 HCAPLUS Full-text
DOCUMENT NUMBER: 147:229603
TITLE: A new bisphosphonate-containing 99mTc(I) tricarbonyl complex potentially useful as bone-seeking agent: synthesis and biological evaluation
AUTHOR(S): Palma, Elisa; Oliveira, Bruno L.; Correia, Joao D. G.; Gano, Lurdes; Maria, Leonor; Santos, Isabel C.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem Codex, 2686-953, Port.
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (2007), 12(5), 667-679
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Aiming to develop new bone-seeking radiotracers based on the organometallic core fac-[99mTc(CO)3]+ with improved radiochem. and biol. properties, we have prepared new conjugates with phosphonate pendant groups. The conjugates comprise a chelating unit for metal coordination, which corresponds to a pyrazolyl-containing backbone (pz) with a N,N,N donor-atom set, and a pendant di-Et phosphonate (pz-MPOEt), phosphonic acid (pz-MPOH) or a bisphosphonic acid (pz-BPOH) group for bone targeting. Reactions of the conjugates with the precursor [99mTc(H2O)3(CO)3]+ yielded (mote than 95%) the single and well-defined radioactive species [99mTc(CO)3(κ3-pz-MPOEt)]+ (1a), [99mTc(CO)3(κ3-pz-MPOH]+ (2a) and [99mTc(CO)3(κ3-pz-BPOH)]+ (3a), which were characterized by

reversed-phase high-performance liquid chromatog. . The corresponding Re surrogates (1-3), characterized by the usual anal. techniques, including X-ray diffraction anal. in the case of 1, allowed for macroscopic identification of the radioactive conjugates. These radioactive complexes revealed high stability both in vitro (phosphate-buffered saline solution and human plasma) and in vivo, without any measurable decomposition Biodistribution studies of the complexes in mice indicated a fast rate of blood clearance and high rate of total radioactivity excretion, occurring primarily through the renal-urinary pathway in the case of complex 3a. Despite presenting moderate bone uptake (3.04 ± 0.47% injected dose per g of organ, 4 h after injection), the high stability presented by 3a and its adequate in vivo pharmacokinetics encourages the search for new ligands with the same chelating unit and different bisphosphonic acid pendant arms.

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2006:711846 HCAPLUS Full-text
DOCUMENT NUMBER: 146:223509
TITLE: Pyrazolyl conjugates of bombesin: A new tridentate ligand framework for the stabilization of fac-[M(CO)3]+ moiety
AUTHOR(S): Alves, Susana; Correia, Joao D. G. ; Santos, Isabel; Veerendra, Bhadrasetty; Sieckman, Gary L.; Hoffman, Timothy J.; Rold, Tammy L.; Figueroa, Said Daibes; Retzloff, Lauren; McCrate, Joseph; Prasanphanich, Adam; Smith, Charles J.
CORPORATE SOURCE: Department of Radiology, University of Missouri-Columbia School of Medicine, Columbia, MO, 65211, USA
SOURCE: Nuclear Medicine and Biology (2006), 33(5), 625-634
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have described the synthesis of tridentate pyrazolyl ligand frameworks for coordination to the fac-[*M(CO)3]+ metal fragment (*M = 186/188Re or 99mTc). These ligands impart a degree of kinetic inertness on the metal center, warranting their study in biol. systems. We herein report in vitro/in vivo radiolabeling investigations of a new series of pyrazolyl bombesin (BBN) conjugates radiolabeled via the Isolink kit. These new conjugates are based on the general structure [99mTc-pyrazolyl-X-BBN[7-14]NH2], where X = β-alanine, serylserylserine or glycylglycylglycine. The pyrazolyl ligand is a tridentate ligand framework that coordinates the metal center through nitrogen donor atoms. The results of these investigations demonstrate the ability of these new conjugates to specifically target the gastrin-releasing peptide receptor subtype 2, which is overexpressed on human prostate PC-3 cancerous tissues. Therefore, these studies suggest the tridentate pyrazolyl ligand framework to be an ideal candidate for the design and development of low-valent 99mTc-based diagnostic radiopharmaceuticals based on BBN or other targeting vectors.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2006:166490 HCAPLUS Full-text
DOCUMENT NUMBER: 145:450851
TITLE: Radiopharmaceuticals for targeted radiotherapy
AUTHOR(S): Marques, Fernanda; Paulo, Antonio; Campello, Maria Paula; Lacerda, Sara; Vitor, Rute Filipe

; Gano, Lurdes; Delgado, Rita; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, Instituto Tecnologico e Nuclear, Sacavem, 2686-953, Port.
SOURCE: Radiation Protection Dosimetry (2005), 116(1-4), 601-604
CODEN: RPDODE; ISSN: 0144-8420
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This work intends to find specific radiopharmaceuticals for cancer therapy based on beta (153Sm and 166Ho) or Auger (99Tcm) emitter radionuclides, using cyclic and acyclic polyamines as bifunctional chelators. These chelators are designed to allow the binding of a tumor seeking biomol. and/or a DNA intercalates. The cyclic amines, such as 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid, 1,4,8,11-tetraazacyclotetradecane-1,4,8,11-tetraacetic acid and 1,4,7,10-tetraazacyclotridecane-1,4,7,10-tetraacetic acid, were radiolabeled with 153Sm and 166Ho. The radiochem. and biol. behavior of the resulting complexes were evaluated in order to assess their potential as building blocks for the attachment of selected biomols., with the aim of further applying them for the development of specific therapeutic radiopharmaceuticals. Novel pyrazolyldiamines, bearing a DNA intercalating anthracenyl fragment, were also explored to synthesize radioactive complexes with the fac-[99Tcm(CO)]3+ moiety. The identity of these 99Tcm tricarbonyl complexes was confirmed by high-performance liquid chromatog. comparison with rhenium congeners fully characterized. By including a DNA intercalator into the chelator framework, we expect to induce more efficient and selective damage to the DNA of cancer cells by the action of the short-range Auger electrons emitted by 99Tcm.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 2005:205084 HCAPLUS Full-text
DOCUMENT NUMBER: 142:406796
TITLE: Pyrazolyl Derivatives as Bifunctional Chelators for Labeling Tumor-Seeking Peptides with the fac-[M(CO)3]+ Moiety (M = 99mTc, Re): Synthesis, Characterization, and Biological Behavior
AUTHOR(S): Alves, Susana; Paulo, Antonio; Correia, Joao D. G.; Gano, Lurdes; Smith, Charles J.; Hoffman, Timothy J.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Bioconjugate Chemistry (2005), 16(2), 438-449
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Radiolabeling of biol. active mols. with the [99mTc(CO)3]+ unit has been of primary interest in recent years. With this in mind, we herein report sym. (L1) and asym. (L2-L5) pyrazolyl-containing chelators that have been evaluated in radiochem. reactions with the synthon [99mTc(H2O)3(CO)3]+ (1a). These reactions yielded the radioactive building blocks [99mTc(CO)3(k3-L)]+ (L = L1-L5, 2a-6a), which were identified by RP-HPLC. The corresponding Re surrogates (2-6) allowed for macroscopic identification of the radiochem. conjugates. Complexes 2a-6a, with log Po/w values ranging from -2.35 to 0.87, were obtained in yields of ≥90% using ligand concns. in the 10-5-10-4 M range. Challenge studies with cysteine and histidine revealed high stability for all of these radioactive complexes, and biodistribution studies in mice indicated a fast rate of blood clearance and high rate of total radioactivity excretion,

occurring primarily through the renal-urinary pathway. Based on the framework of the asym. chelators, the novel bifunctional ligands 3,5-Me2-pz(CH2)2N((CH2)3COOH)(CH2)2NH2 (L6) and pz(CH2)2N((CH2)3COOH)(CH2)2NH2 (L7) have been synthesized and their coordination chemical toward (NEt4)2[ReBr3(CO)3] (1) has been explored. The resulting complexes, fac-[Re(CO)3(k3-L)]Br (L6 (7), L7 (8)), contain tridentate ancillary ligands that are coordinated to the metal center through the pyrazolyl and amine nitrogen atoms, as observed for the other related building blocks. L6 and L7 were coupled to a glycylglycine Et ester dipeptide, and the resulting functionalized ligands were used to prepare the model complexes fac-[Re(CO)3(κ3-3,5-Me2-pz(CH2)2N(glygly)(CH2)2NH2)]+ (9/9a) and fac-[Re(CO)3(κ3-pz(CH2)2N(CH2)3(glygly)(CH2)2NH2)]+ (10/10a) (M = Re, 99mTc). These small conjugates have been fully characterized and are reported herein. On the basis of the in vitro/in vivo behavior of the model complexes (2a-6a, 9a, 10a), we chose to evaluate the in vitro/in vivo biol. behavior of a new tumor-seeking Bombesin pyrazolyl conjugate, [(L6)-G-G-G-Q-W-A-V-G-H-L-M-NH2], that has been labeled with the [99mTc(CO)3]+ metal fragment. Stability, in vitro cell binding assays, and pharmacokinetics studies in normal mice are reported herein.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:639917 HCAPLUS Full-text
DOCUMENT NUMBER: 148:599283
TITLE: Tricarbonyl complexes with tridentate chelators for myocardium imaging
INVENTOR(S): Dos Santos, Isabel da Graca Rego; Paulo, Antonio Manuel Rocha
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 50pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008061792	A2	20080529	WO 2007-EP10216	20071123
WO 2008061792	A3	20080807		

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: GB 2006-23482 A 20061124
OTHER SOURCE(S): CASREACT 148:599283; MARPAT 148:599283

AB Chelators tris(pyrazolyl)methanes (I) and bis(pyrazolyl)amines (II) and (III) (each of R1, R2, R3 and R4 is independently H, linear or branched, (un)saturated C1-9 alkyl; (un)saturated carboxylic group; (un)saturated heterocyclic of heteroaliph. group with 1 or more selected from O, N and S) and Re and 99mTc tricarbonyl complexes of these ligands are reported for use

in myocardial imaging. For example O-methyl-1,1,1-tris(pyrazol-1-yl)ethanol was prepared in a multistep process starting from 2,2,2-tris(pyrazol-1-yl)ethanol and its Re(CO)3 and 99mTc(CO)3 complexes were prepared The biodistribution of the Tc complexes was determined

L34 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:706224 HCAPLUS Full-text
DOCUMENT NUMBER: 147:108440
TITLE: Tripodal ligands with the coordinating motifs κ2-BH2 or κ3-BH3 relevant for biomedical applications of organometallic complexes
INVENTOR(S): Santos, Isabel Rego; Paulo, Antonio Manuel Rocha
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 34pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007073472	A2	20070628	WO 2006-US47877	20061215
WO 2007073472	A3	20070907		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
CA 2634704	A1	20070628	CA 2006-2634704	20061215
EP 1981894	A2	20081022	EP 2006-848716	20061215
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
KR 2008080330	A	20080903	KR 2008-715270	20080623

PRIORITY APPLN. INFO.: EP 2005-77977 A 20051223
EP 2006-75127 A 20060119
WO 2006-US47877 W 20061215
OTHER SOURCE(S): MARPAT 147:108440
AB The present invention relates to a compound for use as a chelator in the radioactive labeling of biomols. with metal tricarbonyl complexes, which compound has the general formula M[BH2RR1] (M = a monovalent cation, such as Li, Na, K, Tl, Rb, Cs or an alkylammonium; R = H, alkyl, aryl or a biomol.; R1 = H or a pendant arm, said pendant arm optionally comprises a biomol., with the proviso that when R = H, R1 is not H or COOH, and when R = alkyl or aryl, R1 is not H). These Mn, Re and Tc carbonyl complexes with [BH2RR1]- can be used in the diagnosis and/or therapy of cancer.

L34 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:722140 HCAPLUS Full-text
DOCUMENT NUMBER: 145:347251

TITLE: Synthesis and biological evaluation of tricarbonyl Re(I) and Tc(I) complexes anchored by poly(azolyl)borates: application on the design of radiopharmaceuticals for the targeting of 5-HT1A receptors
AUTHOR(S): Garcia, Raquel; Gano, Lurdes; Maria, Leonor; Paulo, Antonio; Santos, Isabel; Spies, Hartmut
CORPORATE SOURCE: Departamento de Quimica, ITN, Estrada Nacional 10, Sacavem Codex, 2686-953, Port.
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (2006), 11(6), 769-782
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:347251

AB The building blocks fac-[99mTc{κ3-HB(timMe)3}(CO)3] and fac-[99mTc{κ3-R(μ-H)B(timMe)2}(CO)3] [R is H (4a), Ph (5a); timMe is 2-mercapto-1-methylimidazolyl] were obtained almost quant. by reacting fac-[99mTc(CO)3(H2O)3]+ with the corresponding scorpionate. These compds. cross the intact blood-brain barrier in mice, with significant retention in the case of 4a and 5a. Using 4a as the lead structure, the authors synthesized the functionalized complexes fac-[M{κ3-H(μ-H)B(timBu-pip)2}(CO)3] [M is Re (8), 99mTc (8a); timBu-pip is Me[4-((2-methoxyphenyl)-1-piperazinyl)butyl](2-mercapto-1- methylimidazol-5-yl)methanamide] and fac-[M{κ 3-H(μ-H)B(timMe)(timBu-pip)}(CO)3] [M is Re (9), 99mTc (9a)] and evaluated their potential as radioactive probes for the targeting of brain 5-HT1A serotonergic receptors. The Re complexes exhibit excellent affinity [IC50=0.172 ± 0.003 nM (8); IC50 = 0.65 ± 0.01 nM (9)] for the 5-HT1A receptor. The radioactive congeners (99mTc) showed an initial brain uptake of 1.38 ± 0.46%ID g-1 (8a) and 0.43 ± 0.12%ID g-1 (9a), but suffer from a relatively fast washout.

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:957931 HCAPLUS Full-text
DOCUMENT NUMBER: 147:202224
TITLE: Metal-based drugs for diagnosis and therapy
AUTHOR(S): Alves, Susana; Vitor, Rute; Raposinho, Paula D.; Marques, Fernanda; Correia, Joao D. G.; Paulo, Antonio; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, Instituto Tecnologico e Nuclear, Sacavem, 2686-953, Port.
SOURCE: Metal Ions in Biology and Medicine (2006), 9, 3-8
CODEN: MIBMCT; ISSN: 1257-2535
PUBLISHER: John Libbey Eurotext
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:202224

AB The compound 3,5Me-pz(CH2)2NH(CH2)2NH2 (L1) is a very effective chelator for the fac-[M(CO)3(H2O)3]+ (M = Re (1) 99mTc (1a)) moieties, yielding the building blocks fac-[M(CO)3(k3-L1)]+ (M = Re (2) 99mTc (2a)). The evaluation of the in vitro and in vivo behavior of 2a showed that this stable building block displays a favorable biol. profile for labeling biomols. with 99mTc, biol. active peptides. Due to its versatility, L1 was integrated through its secondary amine into a peptide with affinity for MC1 receptors (L2), and derivatized with an anthracenyl group at the C(4) position of the pyrazolyl

ring (L3). The resulting bifunctional chelators react with 1a yielding the well defined fac-[99mTc(CO)3(k3-L)]+ (L = L2 (3a), L3 (4a)) complexes with excellent stability in vitro and in vivo. Complex 3a presents a significant internalization in B16F1 melanoma cells, showing in vivo a significant overall excretion and a reasonable tumor uptake, with a fast clearance from most organs and tissues. For complex 4a, in vitro studies using B16F1 melanoma cells showed significant nuclear internalization and an enhanced radiotoxicity for this compound, most probably due to the presence of the anthracenyl group which is a known DNA intercalator. The results obtained for complexes 3a and 4a indicate that this family of compds. is potentially useful to develop novel specific 99mTc radiopharmaceuticals directed for both detection and therapy of melanoma.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:902222 HCAPLUS Full-text
DOCUMENT NUMBER: 141:387794
TITLE: Preparation of bifunctional pyrazole -containing tridentate ligands for rhenium and technetium tricarbonyl complexes
INVENTOR(S): Santos, Isabel R.; Galamba Correia, Joao D.; Rocha Paulo, Antonio M.; Alves, Susana; Vitor, Rute
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091669	A1	20041028	WO 2004-US11685	20040415
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1529537	A1	20050511	EP 2003-78217	20031010
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004229568	A1	20041028	AU 2004-229568	20040415
CA 2522326	A1	20041028	CA 2004-2522326	20040415
EP 1644050	A1	20060412	EP 2004-759566	20040415
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1774268	A	20060517	CN 2004-80010214	20040415
JP 2007525452	T	20070906	JP 2006-510091	20040415
US 20060198785	A1	20060907	US 2005-551292	20050928
IN 2005CN02650	A	20070525	IN 2005-CN2650	20051014
NO 2005005334	A	20051111	NO 2005-5334	20051111
PRIORITY APPLN. INFO.:			EP 2003-76106 A	20030415

EP 2003-78217 A 20031010
WO 2004-US11685 W 20040415

OTHER SOURCE(S): MARPAT 141:387794

AB The present invention relates to a chelating agent I [m = 0, 1; X = NR4, S; Y = SR5, NHR5, P(R5)2; R1, R3 = independently H, alkyl, aryl; R2 = H, CO2H, NHR6, (CH2)nCO2R6; R4 = H, alkyl, aryl, (CH2)nCO2R6, (CH2)nOR6; R5 = H, alkyl, aryl, (CH2)nCO2R6, (CH2)nOR6, R6 = H, alkyl, aryl; n = 1-10; when R1 = R3 = CH3, R2, R4, R5 are not all = H]. The invention further relates to a method and kit for the preparation of radiolabeled biomols. while using the chelating agent. Thus, pyrazole II (R = CO2H) was prepared by cyclocondensation of (OHC)2CHCO2Et with H2NNHCH2CH2OH, followed by tosylation and substitution with ethylenediamine and saponification Prepared compds. II (R = H, CO2H) underwent complexation with rhenium and technetium-99 to give the corresponding tricarbonyl complexes.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1049014 HCAPLUS Full-text

DOCUMENT NUMBER: 142:168330

TITLE: Rhenium(I)- and technetium(I) tricarbonyl complexes anchored by bifunctional pyrazole -diamine and pyrazole-dithioether chelators

AUTHOR(S): Vitor, Rute F.; Alves, Susana; Correia, J. D. G.; Paulo, Antonio; Santos, Isabel

CORPORATE SOURCE: ITN, Estrada Nacional, Departamento de Quimica, Sacavem Codex, 2686-953, Port.

SOURCE: Journal of Organometallic Chemistry (2004), 689(25), 4764-4774
CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:168330

AB The novel pyrazolyl containing ligands 4-(HOOC)pz(CH2)2NH(CH2)2NH2 (L1) and 4-(HOOCCH2)-3,5-Me2pz(CH2)2NH(CH2)2NH2 (L2), and 3,5-Me2pz(CH2)2S(CH2)2SCH2CH3 (L3), 3,5-Me2pz(CH2)2S(CH2)2SCH2COOEt (L4) and 3,5-Me2pz(CH2)2S(CH2)2SCH2COOH (L5) were synthesized, and their ability to stabilize complexes with the fac-[M(CO)3]+ (M = Re,99mTc) moiety was evaluated. Reactions of L1-L5 with (NEt4)2[Re(CO)3Br3] and/or [Re(CO)5Br] afforded complexes fac-[Re(CO)3(κ3-L)] (L = L1-L5 (1-5)), which contain the pyrazolyl ancillary ligands coordinated in a tridentate fashion. Complexes 1-5 were characterized by the common anal. techniques, which included single crystal x-ray diffraction anal. in the case of 4. The structural anal. of 4 confirmed the tridentate coordination mode of the pyrazole-dithioether ligand, which is facially coordinated to the Re(I) center through the N from the pyrazole ring and the two thioether S atoms, without involvement of the terminal ester functional group. The distorted octahedral coordination environment around the metal is completed by the three facial carbonyl ligands. The radioactive congeners of complexes 1, 3 and 4, fac-[99mTc(CO)3(κ3-L)]+ (L = L1 (1a), L3 (3a), L4 (4a)), were prepared by reacting the precursor fac-[99mTc(CO)3(H2O)3]+ with the corresponding ligands, and their identity confirmed by HPLC comparison with the Re surrogates. Complexes 1a and 3a were challenged in the presence of a large excess of histidine or cysteine, to evaluate their in vitro stability. Only a negligible displacement was observed, indicating that pyrazole-diamine and pyrazole-dithioether chelators provide a high kinetic inertness and/or stability to organometallic complexes with the fac-[99mTc(CO)3]+ moiety.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:937047 HCAPLUS Full-text
DOCUMENT NUMBER: 138:330675
TITLE: Coordination capabilities of pyrazolyl containing ligands towards the fac-[Re(CO)3]+ moiety
AUTHOR(S): Alves, Susana; Paulo, Antonio; Correia, Joao D. G.; Domingos, Angela; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Journal of the Chemical Society, Dalton Transactions (2002), (24), 4714-4719
CODEN: JCSDAA; ISSN: 1472-7773
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:330675
AB The coordination capabilities of the pyrazolyl containing ligands pz*(CH2)2NH(CH2)2pz*, pz*(CH2)2NH(CH2)2NH2, pz*(CH2)2S(CH2)2pz* and pz*(CH2)2S(CH2)2NH2 (pz* = 3,5-Me2pz) towards the synthon (NEt4)2[ReBr3(CO)3] (1) were studied. Depending on the reaction conditions, neutral or cationic Re(I) tricarbonyl complexes were isolated: [ReBr(CO)3(κ2-pz*(CH2)2NH(CH2)2pz*)] (2), [ReBr(CO)3(κ2-pz*(CH2)2S(CH2)2pz*)] (3) [Re(CO)3(κ3-pz*(CH2)2NH(CH2)2pz*)]Br (4), [Re(CO)3(κ2-pz*(CH2)2S(CH2)2pz*)MeOH]Br (5), [Re(CO)3(κ3-pz*(CH2)2NH(CH2)2NH2)]Br (6) and [Re(CO)3(κ3-pz*(CH2)2S(CH2)2NH2)]Br (7). Complexes 2-7 were characterized by the normal techniques, including x-ray crystallog. anal. in the case of 3, 4, 6 and 7. In these complexes the Re atom adopts a distorted octahedral coordination, being one of the triangular faces defined by the three carbonyl groups and the other three remaining coordination positions by the bidentate and the bromide ligands (3), or by the tridentate and neutral pyrazolyl containing ligands (4, 6, 7). Complexes 2-4, 6 and 7 are static in solution and the 1H NMR data indicate clearly a κ2-coordination mode of the ligand in 2 and 3 and a κ3-coordination in 4, 6 and 7, which agrees with the coordination mode found in the solid state. Compound 5 displays a fluxional behavior in solution as shown by variable temperature 1H NMR studies. No x-ray data exists for this complex but the pattern obtained for the NMR spectrum at 215 K indicates a κ2-coordination mode for the pyrazolyl containing ligand.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:688342 HCAPLUS Full-text
DOCUMENT NUMBER: 132:101913
TITLE: Control of the hapticity of pyridine-2-thiolate ligands in rhenium(V) oxo complexes
AUTHOR(S): Paulo, Antonio; Domingos, Angela; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, Estrada Nacional 10, ITN, Sacavem, 2686-593, Port.
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1999), (21), 3735-3740
CODEN: JCDTBI; ISSN: 0300-9246
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Treatment of [ReO{κ3-B(pz)4}(OMe)2] 1 (B(pz)4 = tetrapyrazolylborate) with pyridine-2-thiol ligands led to [ReO{κ2-B(pz)4}(κ2-Spy*)(OMe)] (Spy* = 2-

SC5H4N 2 or 2-SC5H3NSiMe3-3 3) or [ReO{κ3-B(pz)4}(κ1-2-SC5H4N)2] 4, depending on the reaction conditions. Complexes 2 and 3 reacted with trimethylsilyl chloride yielding [ReO{κ3-B(pz)4}(κ1-2- SC5H4N)Cl]·HCl 6 and [ReO{κ3-B(pz)4}Cl2], resp. The characterization of the new compds. involves IR and 1H NMR spectroscopies, x-ray diffraction anal. for 3, 4 and 6.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 15 OF 15 EMBASE COPYRIGHT (c) 2008 Elsevier B.V. All rights reserved on STN

ACCESSION NUMBER: 2005304949 EMBASE Full-text

TITLE: Life-threatening ventilatory obstruction due to a defective tracheal tube during spinal surgery in the prone position [8] (multiple letters).

AUTHOR: Santos, Isabel A., Dr. (correspondence)

CORPORATE SOURCE: Hospital Geral de Santo Antonio, Porto, Portugal. ialex@mail.telepac.pt

AUTHOR: Bertaggia, Gregor

CORPORATE SOURCE: Tyco Healthcare, Hennef, Germany. gregor.bertaggia@emea.tycohealthcare.com

AUTHOR: Oliveira, Carla A.; Ferreira, Leonia; Kennedy, Deirdre

SOURCE: Anesthesiology, (Jul 2005) Vol. 103, No. 1, pp. 214-215. ISSN: 0003-3022 CODEN: ANESAV

COUNTRY: United States

DOCUMENT TYPE: Journal; Letter

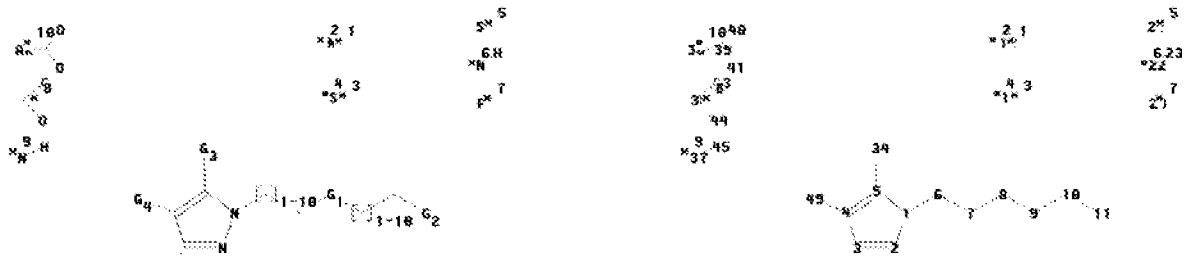
FILE SEGMENT: 024 Anesthesiology
027 Biophysics, Bioengineering and Medical Instrumentation
037 Drug Literature Index
009 Surgery

LANGUAGE: English

ENTRY DATE: Entered STN: 29 Sep 2005
Last Updated on STN: 29 Sep 2005

Structures uploaded into STN REGISTRY

Uploading L1.str



chain nodes :
6 7 8 9 10 11 21 22 23 24 33 34 36 37 38 39 40 41 43 44 45 49

ring nodes :
1 2 3 4 5
ring/chain nodes :
12 13
chain bonds :
1-6 3-33 4-49 5-34 6-7 7-8 8-9 9-10 10-11 22-23 36-43 36-44 37-45 38-39
39-40 39-41
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-6 2-3 3-4 3-33 4-5 4-49 5-34 6-7 7-8 8-9 9-10 10-11 36-43
36-44 37-45 38-39 39-40 39-41
exact bonds :
22-23

G1:[*1-*2],[*3-*4]

G2:[*5],[*6],[*7]

G3:H,Cb,Ak

G4:[*8],[*9],[*10]

Hydrogen count :
3:>= minimum 0
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS
11:CLASS 12:CLASS 13:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 33:CLASS
34:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 43:CLASS 44:CLASS 45:CLASS
49:CLASS

Full search history

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=> d his full

     (FILE 'HOME' ENTERED AT 10:16:23 ON 16 DEC 2008)

     FILE 'REGISTRY' ENTERED AT 10:16:36 ON 16 DEC 2008
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L3          12 SEA SSS FUL L1
               D SCAN
               SAVE L3 SCH292L1ST/A

     FILE 'HCAPLUS' ENTERED AT 10:19:08 ON 16 DEC 2008
L4           5 SEA SPE=ON  ABB=ON  PLU=ON  L3
               D L4 1-5 TI
               D L4 1-5 AU
               SAVE L4 SCH292HCST/A
               E SANTOS I?/AU
L5         483 SEA SPE=ON  ABB=ON  PLU=ON  SANTOS I?/AU
               E CORREIA J?/AU
L6         527 SEA SPE=ON  ABB=ON  PLU=ON  CORREIA J?/AU
               E PAULO A?/AU
L7          91 SEA SPE=ON  ABB=ON  PLU=ON  PAULO A?/AU
               E ALVES S?/AU
L8         324 SEA SPE=ON  ABB=ON  PLU=ON  ALVES S?/AU
               E VITOR R?/AU
L9          20 SEA SPE=ON  ABB=ON  PLU=ON  VITOR R?/AU
L10          2 SEA SPE=ON  ABB=ON  PLU=ON  L5 AND L6 AND L7 AND L8 AND L9
L11         56 SEA SPE=ON  ABB=ON  PLU=ON  L5 AND (L6 OR L7 OR L8 OR L9)
L12         12 SEA SPE=ON  ABB=ON  PLU=ON  L6 AND (L7 OR L8 OR L9)
L13          8 SEA SPE=ON  ABB=ON  PLU=ON  L7 AND (L8 OR L9)
L14          3 SEA SPE=ON  ABB=ON  PLU=ON  L8 AND L9
L15       1366 SEA SPE=ON  ABB=ON  PLU=ON  (L5 OR L6 OR L7 OR L8 OR L9)
L16          3 SEA SPE=ON  ABB=ON  PLU=ON  L15 AND MALLINCKRODT?/CO,CS,PA,SO
L17         57 SEA SPE=ON  ABB=ON  PLU=ON  (L11 OR L12 OR L13 OR L14)
L18         32 SEA SPE=ON  ABB=ON  PLU=ON  L17 AND PYRAZOL?
L19         28 SEA SPE=ON  ABB=ON  PLU=ON  L17 AND (TRICARBON? OR TRIDENT?)
L20          5 SEA SPE=ON  ABB=ON  PLU=ON  L10 OR L16
L21         49 SEA SPE=ON  ABB=ON  PLU=ON  L18 OR L19
L22         11 SEA SPE=ON  ABB=ON  PLU=ON  L18 AND L19
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               D STAT QUERY L4

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                D L26
L27             STRUCTURE UPLOADED
                D L27

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L28           0 SEA SUB=L3 SSS SAM L27
L29           2 SEA SUB=L3 SSS FUL L27
                D L29
                D SCAN
                SAVE L29 SCH292L27ST/A
L30          12 SEA SPE=ON  ABB=ON  PLU=ON  L3 OR L29
                D SCAN

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L31           5 SEA SPE=ON  ABB=ON  PLU=ON  L30
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                D QUE L24
                D QUE L25

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L34          15 DUP REM L23 L25 (15 DUPLICATES REMOVED)
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                     ANSWER '15' FROM FILE EMBASE
                D L34 1-15 IBIB AB


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   14 DEC 2008  HIGHEST RN 1084385-33-0
     DICTIONARY FILE UPDATES:  14 DEC 2008  HIGHEST RN 1084385-33-0

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     predicted properties as well as tags indicating availability of
     experimental property data in the original document.  For information
     on property searching in REGISTRY, refer to:

     http://www.cas.org/support/stngen/stndoc/properties.html

     FILE HCAPLUS

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FILE COVERS 1907 - 16 Dec 2008 VOL 149 ISS 25
FILE LAST UPDATED: 15 Dec 2008 (20081215/ED)

HCAplus now includes complete International Patent Classification (IPC)
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MEDLINE Accession Numbers (ANs) for records from 1950-1977 have
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searched, and displayed in all records from 1949 to the present.

FILE BIOSIS
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CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
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BIOSIS has been augmented with 1.8 million archival records from 1926
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FILE EMBASE
FILE COVERS 1974 TO 16 Dec 2008 (20081216/ED)

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